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A REVIEW ON DERIVATIVE SPECTROSCOPY AND ITS BENEFITS IN DRUG ANALYSIS

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ABSTRACT

Derivative UV spectrophotometry is an analytical technique used in multi component analysis. It has enormous implication commonly in obtaining mutually qualitative and quantitative in order from spectra that are of unresolved bands, with respect to qualitative and quantitative analysis, it uses first or higher derivatives of absorbance in accordance with wavelength. [1] Derivative spectroscopy is the simplest method for an increasing selectivity is derivatization of spectra. This method is used when the sample of drug shows large irrelevant absorption. It involves conversion of normal spectrum to its first, second and higher derivative spectra where its amplitude in the derivative spectrum is proportional to the concentration of the analyte provided that Beer's law is obeyed by the fundamental spectrum. This article provides you a clear view of derivative spectroscopy and its advantages and disadvantages in analysis of the sample.

Key words: Derivative spectroscopy, Spectra, Wavelength, First, second and third order spectra.

INTRODUCTION:

The term derivative spectrum refers to spectral measurement technique in which the slope of the spectrum i.e., rate of change of absorbance with wavelength, is measured as a function of the wavelength. Thus first derivative spectrum is the plot of spectral slope against wavelength and the second derivative is itself the derivative of first derivative spectrum (figure 1). We will illustrate this by using zero order spectrum. It is the fundamental spectrum. It increases selectivity by derivatization of set of digital data and also by removing spectral interferences [4].

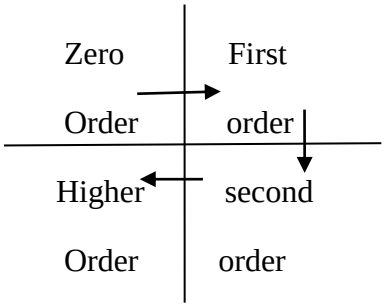

Figure 1 : Zero, first, second and higher order derivatives

HISTORY:

Derivative spectroscopy is brought up in 1950s with its applicability in lot of features, but because of its complication in producing derivative spectrum in UV spectroscopy the method found less in practice. The first analogue spectroscopy was built by Singleton and Cooler. It increases selectivity by derivatization of set of digital data and also by removing spectral interferences. In 1970s with the use of microcomputers derivative spectra became more specific, simple, rapid and reproducible way. This made to enlarge applicability of derivative method; Derivatization of spectra augments selectivity by eradicates spectral interferences [2-3]. Mathematical derivative of absorbance with respect to wavelength of radiation is calculated by the instrument itself, electronically or by using microcomputer.

DERIVATIVE SPECTROSCOPY:

It is a spectroscopic technique that differentiates spectra's mainly in IR, UV-Visible absorption and fluorescence spectrometry. The objective with which derivative methods used in analytical chemistry are:

- Spectral differentiation
- Spectral resolution enhancement
- Quantitative analysis

SPECTRAL DIFFERENTIATION

It is a qualitative method of spectrum that distinguishes small variations between almost similar spectra's.

SPECTRAL RESOLUTION ENHANCEMENT

Overlapping spectral bands gets resolved to simply estimation the number of bands and their wavelengths.

QUANTITATIVE ANALYSIS

It facilitates multicomponent analysis and corrects the irrelevant background absorption. Derivative spectroscopy method forms the beginning of differentiation or resolution of overlapping bands [7]. The vital characteristics of derivative process are that broad bands are suppressed relative to sharp bands.

ZERO, FIRST, AND HIGHER ORDER DERIVATIVES:

In derivative spectroscopy the ability to detect and to measure minor spectral features is considerably enhanced. This enhancement of characteristic spectral detail can distinguish very similar spectra and follow subtle changes in spectrum. Moreover, it can be of use in quantitative analysis to measure the concentration of an analyte whose peak is obscured by a larger overlapping peak due to something else in the sample. Let us consider an example (figure 2), one cannot draw a unique tangential baseline, but if a

reasonable guess is made, the reading of 0.4 is far too low. Referring to the derivative spectra in the lower right of (Figure 2), one can take as the measure of the analyte intensity the vertical distance between the adjacent maximum and minimum of the first derivative, Now our estimate of the analyte intensity is low by only 12%. Whenever the interfering band is at least a factor of 2 boarder than the analyte band, it will usually be advantageous to base the measurement on the derivative spectra [5]

Note: The derivative spectra are more structured than the original spectra, since the number of peaks goes on increasing with increase in the order of derivative. In the first order, original band splits into two. In the second order, original band splits into three. Thus the number of peaks in a spectrum of order 'n' would be [4]

n = (n+1)

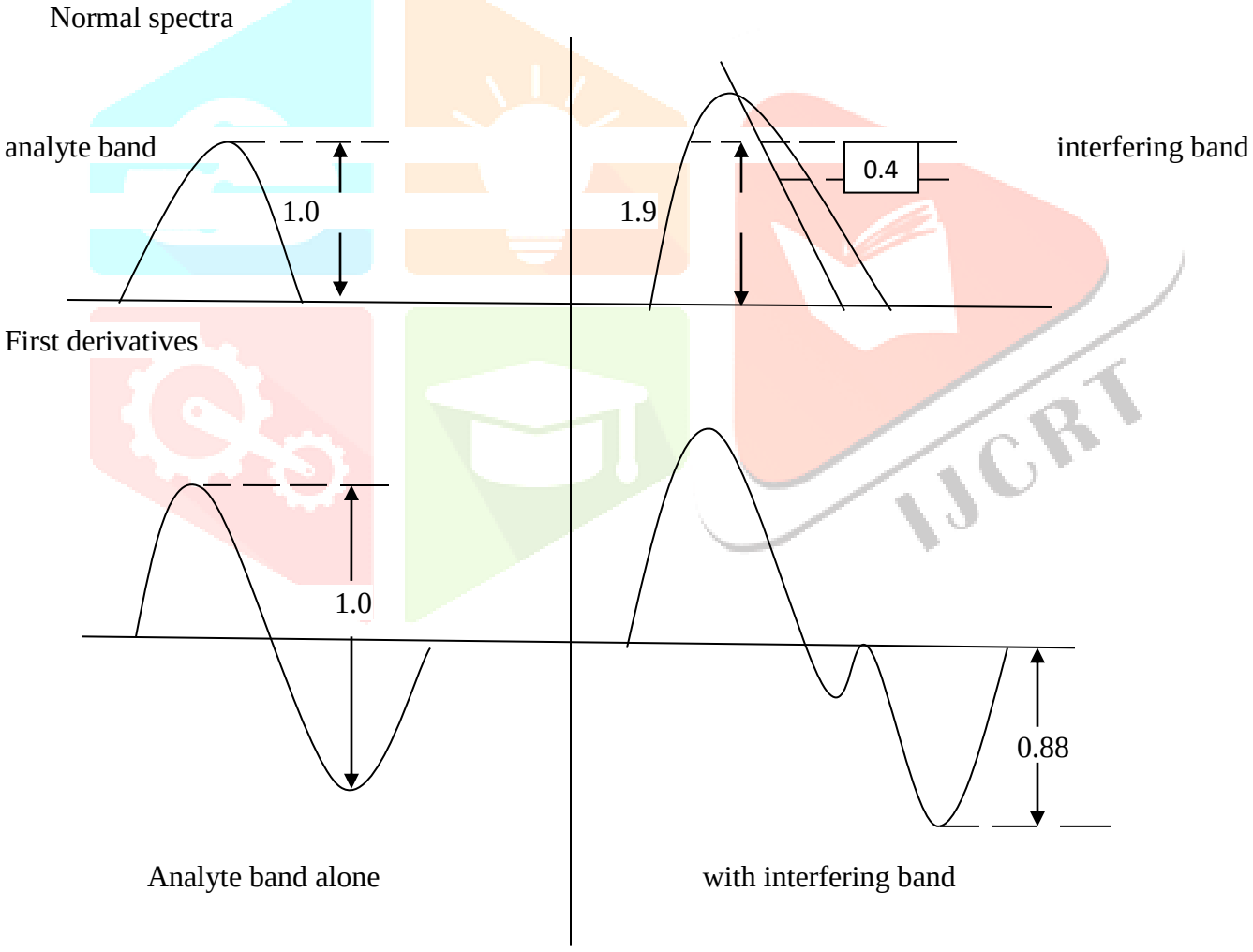

Figure 2 First derivative spectrometry for the quantitative measurement of intensity of a small band (analyte band) and (interfering band) obscured by a boarder overlapping band [2]

Zero order spectrum is the fundamental spectrum i.e absorbance vs wavelength. A first-order derivative is the rate of change of absorbance with respect to wavelength. A first- order derivative starts and finishes at zero. It also passes through zero at the same wavelength as A_{max} of the absorbance band. Either sides of these points

are positive and negative bands with maximum and minimum at the same wavelengths as the inflection points in the absorbance band. This bipolar function is characteristic of all the order derivatives. Thus, first order spectrum or D^0 Spectrum is calculated as

dA/d□□□

The second order spectrum is the plot of curvature of D^0 spectrum against wavelength. The most characteristic feature of a second-order derivative is a negative band with minimum at the same wavelength as the maximum on the zero-order band (figure 4). It also shows two additional positive satellite bands either side of the main band. Those satellite bands are cross over points in D^2 spectrum (figure 4).

$D^2A/d□^□$

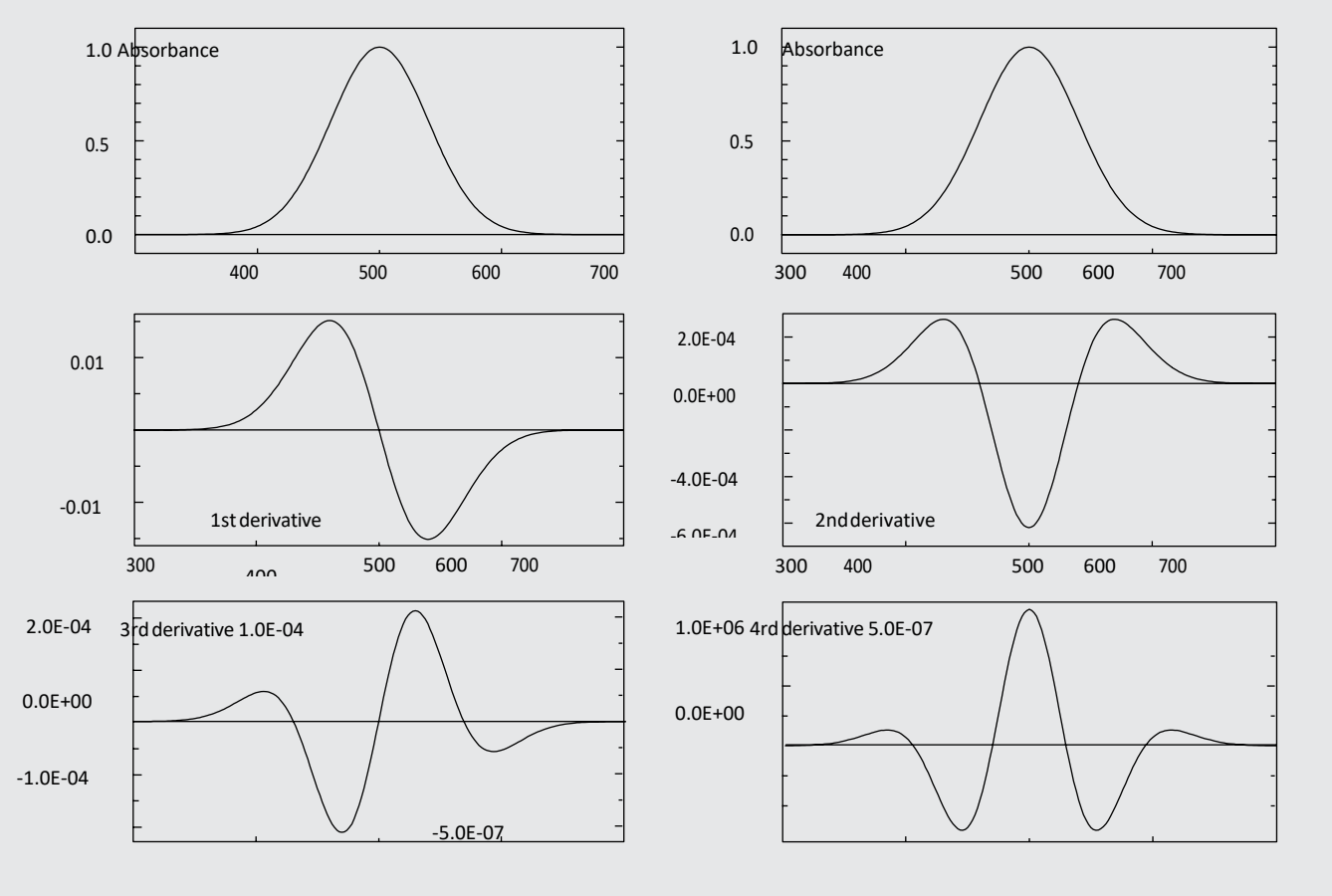

Figure 3: Absorption bands of zero, first, second and higher derivative spectrum[6]

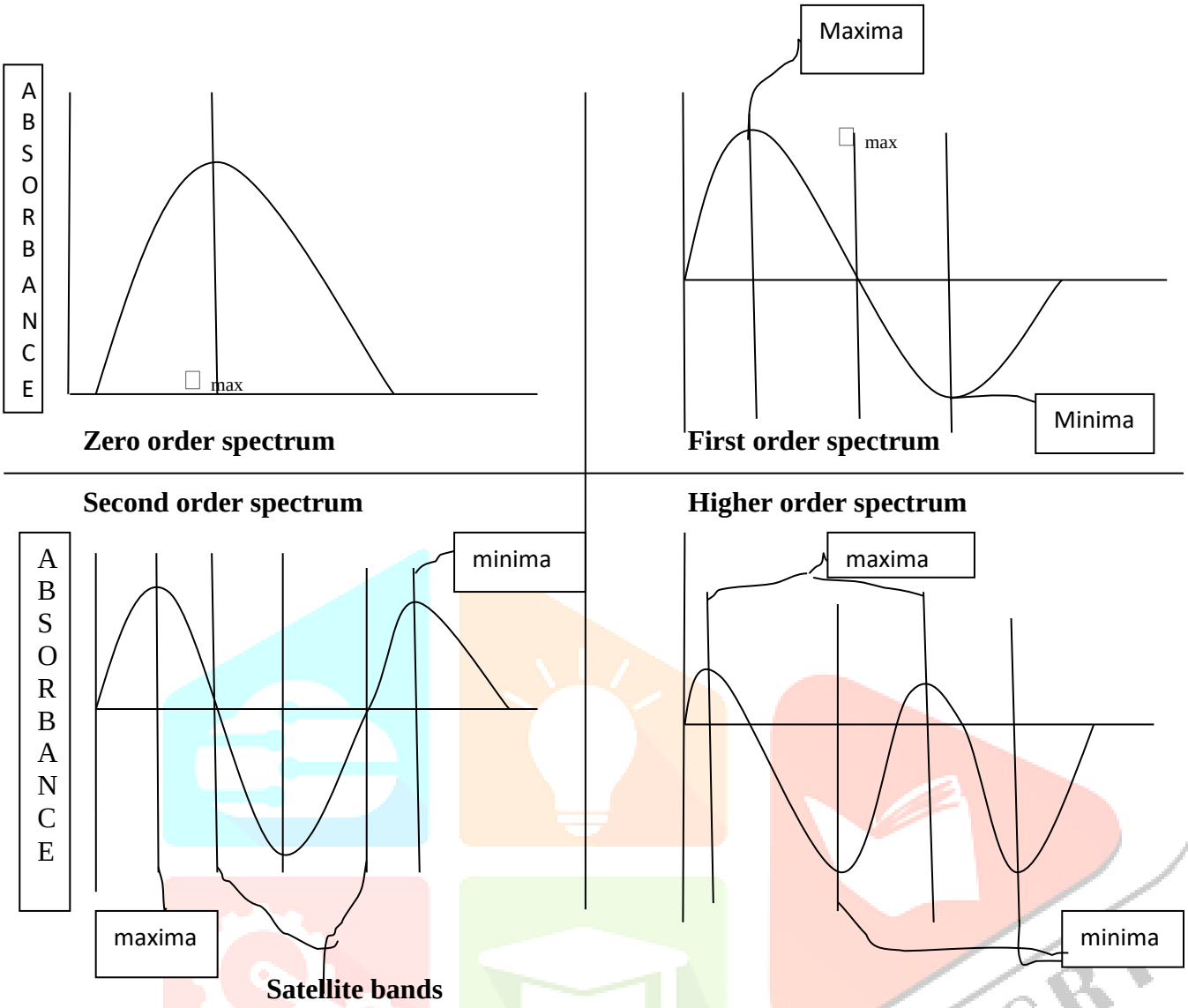

Figure 4: representing the maxima and minima of the spectrum (zero, first, second and higher order derivatives)[4]

Amplitude of the peak can be calculated by $(1/w)^n$. where w is peak width and n is the order of the derivative of the spectrum.

Obtaining derivative spectra

Derivative spectra can be obtained by optical, electronic, or mathematical methods. Optical and electronic techniques were used on early UV-Visible spectrophotometers but have largely been superseded by mathematical techniques. The advantages of the mathematical techniques are that derivative spectra may be easily calculated and recalculated with different parameters and smoothening techniques maybe used to improve signal to noise ratio [6]

USES OF DERIVATIVE SPECTROSCOPY

The advantages of the derivative spectroscopy is an even order spectrum is of narrower spectral bandwidth than its fundamental spectrum. A derivative spectrum shows better resolution of overlapping bands than the fundamental spectrum and may permit the accurate determination of the □ max of the individual bands. Even in small wavelength range, in presence of two or more overlapped peaks, absorbance bands can be identified. Background effect can be eliminated in derivative spectra. It is simple and cost effective method. It gives quick, easy and reproducible date. Selectivity without separation of analyte. Improves sensitivity and specificity. It is faster than classical techniques and can be used where classical techniques are not applicable.

The main disadvantage of derivative spectroscopy is its dependence on instrumental parameters like speed of scan and the slit width. The instrumental conditions of recording parent zero-order spectrum have strong influence on the shape and intensity of its derivative generations.

CONCLUSION:

Derivative spectroscopy makes easy for the analyst in obtaining useful information from the spectra of compounds. It is completely based on the instrument. This article provides you the information about derivative spectroscopy.

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